NIST
National Institute of Standards and Technology

Polymer Formulations

Multivariant Measurement Methods Group

Project 1

Leader: Kate Beers

Polymer Formulations

Complex mixtures with multiple component types

Personal Care: $ 26 billion◘ (1999)
Detergents: $ 4.7 billion* (1999)
Fabric Softener: $ 1.3 billion* (1999)
Coatings: $ 21.2 billion** (2000)

◘ Kline and Co.
*Information Resources Inc.
** PGPhillips and Assoc.

"Getting the ingredients and proportions right is a matter of experience if formulators are using tried-and-true ingredients or trial and error if they are moving in new directions. They need to end up with a formulation that has all of the desired attributes for the consumer as well as being processible, stable, and within budget."

C&EN, April 15, 2002

NCMC Meeting: Spring 2002

Open Discussion on Formulations

Member companies:

- Air Products & Chemicals
- Akzo Nobel
- BASF
- Bayer
- Exxon-Mobil
- Gillette
- Procter & Gamble
- Rhodia, Inc.
- Rohm and Haas

New members:

- 3M
- ICI (National Starch)
- Honeywell International
- Air Force Research Labs

Properties:

- Disperisivity
- Stability
- Viscosity
- Surface Tension
- Rheology
- Homogeneity
- Turbidity

Variables:

- H_2O (hardness, pH, humidity, etc.)
- Molecular weight
- Temperature
- Time
- UV-exposure
- Order and methods of mixing

NEW PROJECT: Polymer Formulations

Objective: To develop HT or combinatorial methods for measuring properties, such as viscosity, interfacial tension, wettability, compatibility and reactivity, of polymeric mixtures involving multiple component types

Problem: How to design systematic approaches to measure the many complex, poorly understood interactions presently addressed with little more than empirical knowledge?

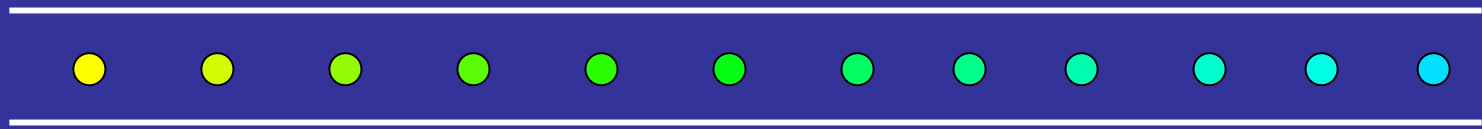
Approach: Develop *modular, rapid and small scale* fluidic reactors, mixing devices and measurement techniques

Focus: Emulsions using polymeric surfactants

Fluidics: A paradigm shift for the COMBI group

Dynamic sample libraries with
- time dependent composition variations
- both interval and gradient coverage of parameter space

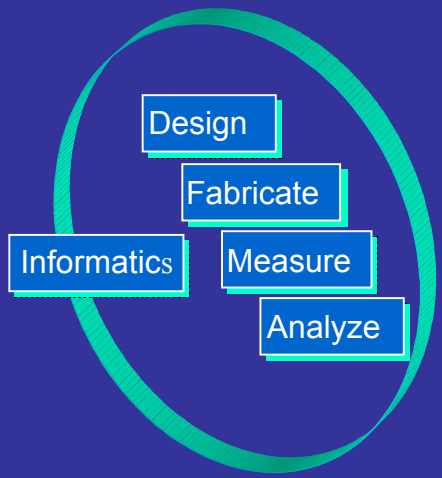
Systematic variation in droplet composition:

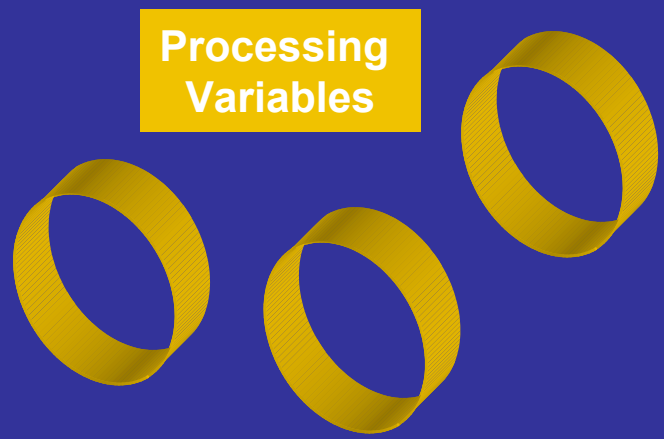


Measurements to serve as feedback for
- each sequence of mixing or reacting
- the final complex mixture of components (water, oil phase + surfactant)

INFORMATICS (and possibly DOE) will be critical to development of processes

Modular Libraries





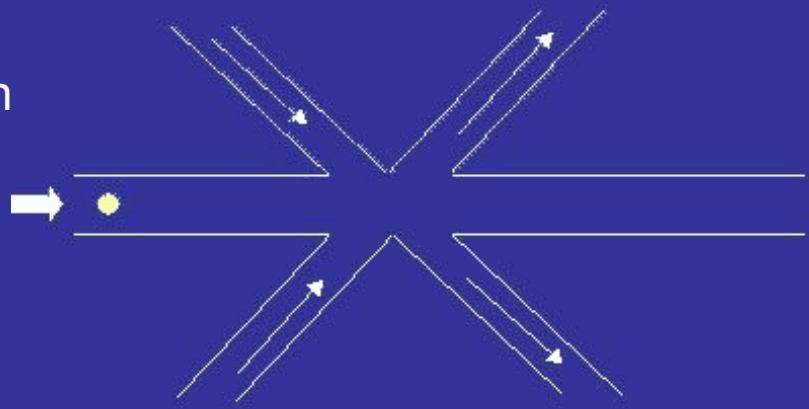
Fluidic Device Examples

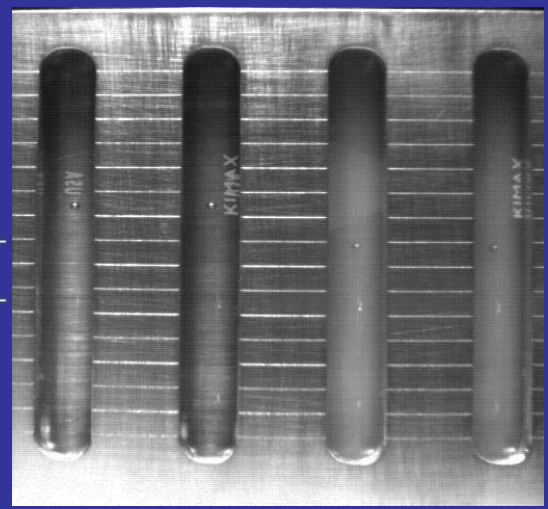
Initial variables:

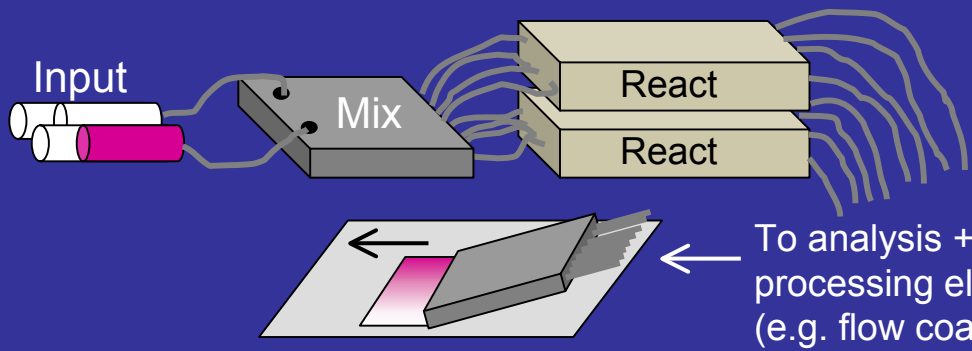
- Molecular parameters of additives (block and statistical copolymers)
- Composition of emulsion droplets (oil phase)

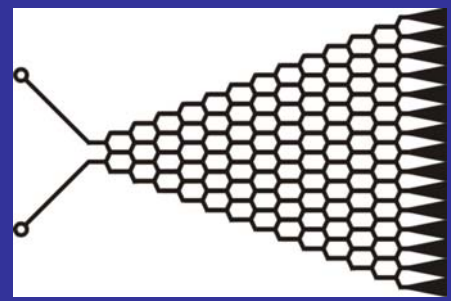
Initial properties:

- Interfacial Tension
- Stability
- Viscosity

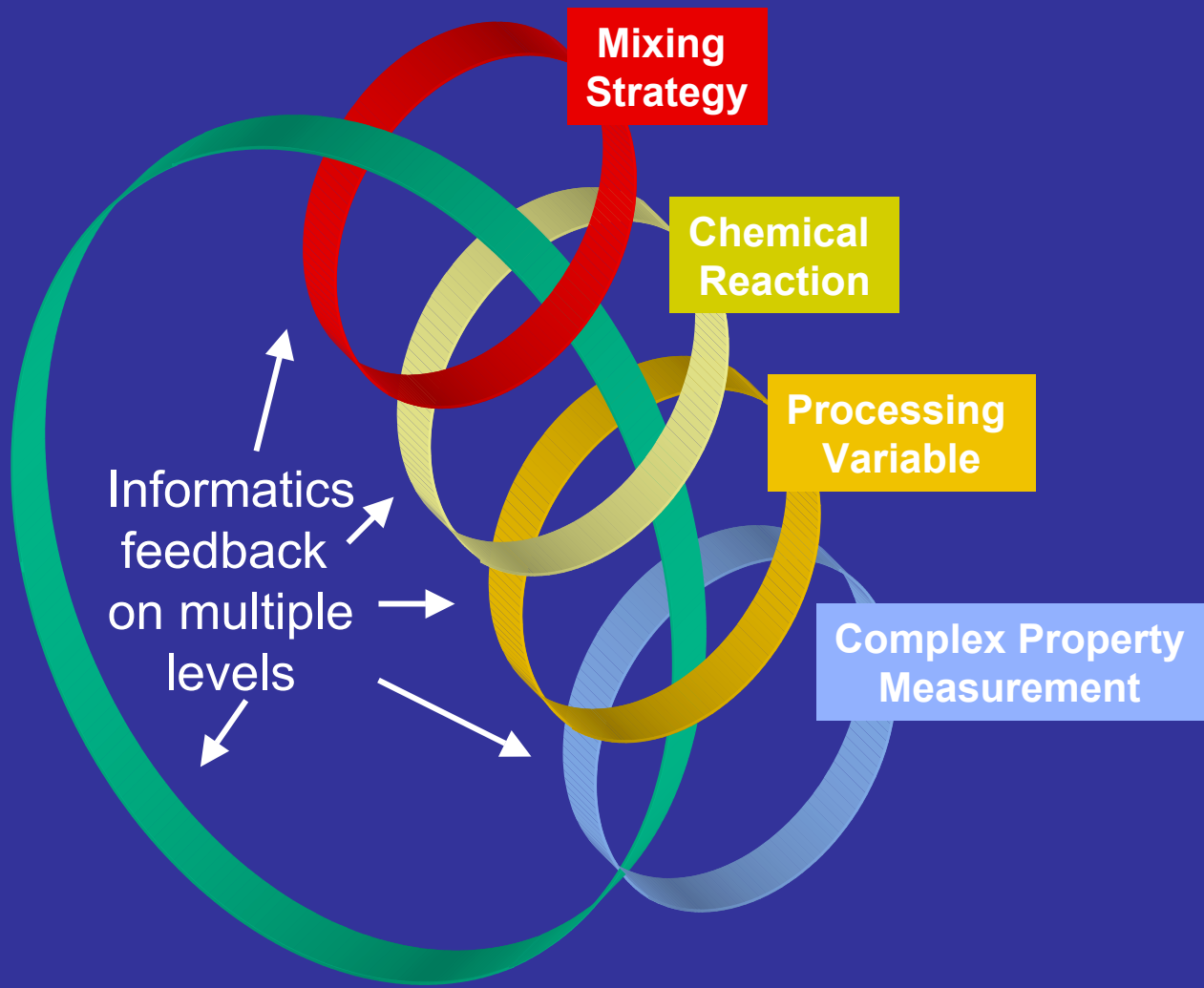








Designing a Process



Formulations Team

Polymers Division:

- K. Beers (Project Leader; reactive systems, gradient synthesis)
- J. Cabral (Guest Researcher; mixing strategies)
- H. Walls (NRC Postdoc; rheology)
- S. Hudson (micro- and nanoscale manufacturing project)
- C. Stafford (NRC Postdoc; mixing strategies)
- J. Douglas (theory and modeling)

Potential Collaborators:

- NCMC Focus Project: Interfacial Tension (Procter and Gamble, Rhodia, etc.)
- MEL: Precision Engineering (John Dagata)
- CSTL: Physical and Chemical Properties (?)